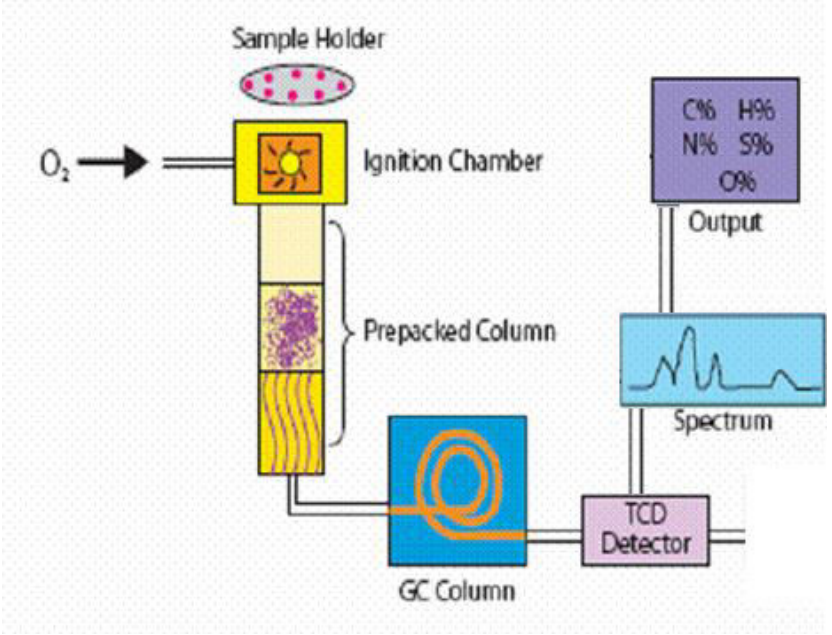
Chapter 3
Empirical and Molecular Formula

- **Empirical formula** is the simplest formula for a compound that give the proportions of the elements present in a compound but not the actual numbers or arrangement of atoms.

- **Molecular formula** is the same as empirical formula or its multiple, and it give the actual number of atoms in the compound.

- For example, if the molecular formula of a compound is C_4H_{10}, it has only one empirical formula = C_2H_5
- If the empirical formula of a compound is C_3H_8, its molecular formula may be C_3H_8 , C_6H_{16} , etc.

• The data needed to calculate the empirical and molecular formula can be obtained from a chemical test called elemental analysis.



How to calculate the empirical formula?

Q- a compound is found to contain the following % by mass: 69.58% Ba, 6.090% C, 24.32% O. What is the simplest (or empirical) formula?

Step 1: imagine that you have 100 g of the substance. Thus, % will become mass in grams. E.g. 69.58 % Ba becomes 69.58 g Ba. (Some questions will give grams right off, instead of %)

Step 2: calculate the # of moles (mol = g ÷ g/M.Wt)

Ba:	69.58 g	÷	137.33 g/mol	=	0.507 mol Ba
C:	6.090 g	÷	12.01 g/mol	=	0.507 mol C
O:	24.32 g	÷	16.00 g/mol	=	1.52 mol O

Step 3: express moles as the simplest ratio by dividing through by the lowest number.

mol	**Ba**	**C**	**O**
	0.507	0.507	1.52
mol (reduced)	0.507/ 0.507 = 1	0.507/ 0.507 = 1	1.52/ 0.507= 3

Step 4: write the simplest formula from mol ratios:

The simplest formula is $BaCO_3$

Mole ratios and simplest formula

Given the following mole ratios for the hypothetical compound AxBy, what would x and y be if the mol ratio of A and B were:

A = 1 mol, B = 2.98 mol	AB_3
A = 1.337 mol, B = 1 mol	A_4B_3
A = 2.34 mol, B = 1 mol	A_7B_3
A = 1 mol, B = 1.48 mol	A_2B_3

Practical Exercises

1. A compound consists of 29.1 % Na, 40.5 % S, and 30.4 % O. Determine the simplest formula.

2. A compound is composed of 7.20 g carbon, 1.20 g hydrogen, and 9.60 g oxygen. Find the empirical formula for this compound.

The molar mass (g/mol) of Na = 22.99, S = 32.06 , O = 16.00, C = 12.01, H = 1.01

Molecular formula calculations

- To find the molecular formula, you need the molar mass of the compound.
- In question 2, if the molecular mass of the compound is 150 g/mol, what is the molecular formula??
- First calculate the molecular mass of CH_2O which is 30 g/mol (12+2+16).
- Divide the molar mass of the compound by this to get a factor: 150 g/mol ÷ 30 g/mol = 5
- Multiply each subscript in the formula by this factor: $C_5H_{10}O_5$ is the molecular formula.

Ex. Solve each of the following:

1- Combustion analysis gives the following percentages: 26.7% C, 2.2% hydrogen, 71.1% oxygen. If the molecular mass of the compound is 90 g/mol, determine its molecular formula.

2- A compound's empirical formula is CH, and it weighs 104 g/mol. Give the molecular formula.

3- A substance is decomposed and found to consist of 53.2% C, 11.2% H, and 35.6% O by mass. Calculate the molecular formula of the unknown if its molar mass is 90 g/mol.

Draw one possible molecular structure for each molecular formula for each example